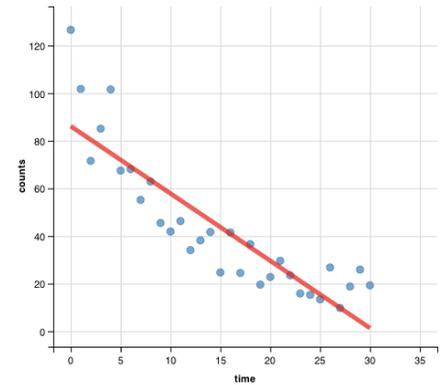


Activity #12: More regression topics: Polynomial, robust, quantile regression; lowess; ANOVA as regression

Scenario: 31 counts (over a 30-second period of time) were recorded from a Geiger counter at a nuclear plant:

	Time	Count (above background radiation levels)	
	0	126.6	
	1	101.8	
	2	71.6	
	...	...	
	30	19.3	
=====			
Mean =	15	43.745	N = 31
SD =	9.09	29.308	r = -0.877



- Based on the correlation (or the R-squared value of 0.7687), we might feel satisfied that a linear model adequately fits this data (predicting counts as a function of time). Based on the following residual plots, evaluate the conditions for a linear regression model:

**Model: count =  $b_0 + b_1(\text{time})$**

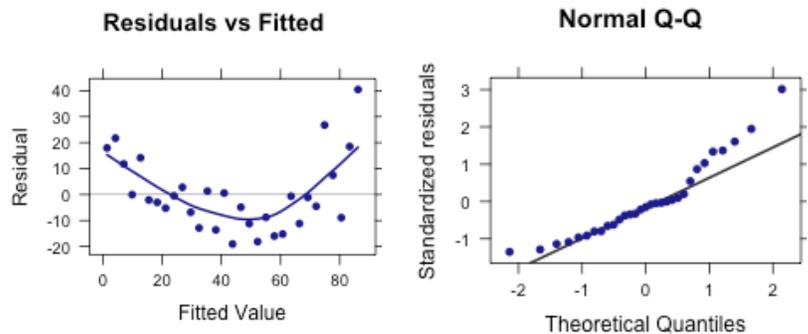
Least-squares line:  $y = 86.14 - 2.826x$

$R^2 = 0.7687$

RMSE = 14.34

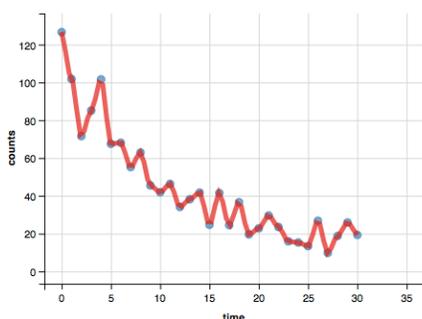
AIC = 256.996

F = 96.397 ( $p = 9.991e-11$ )

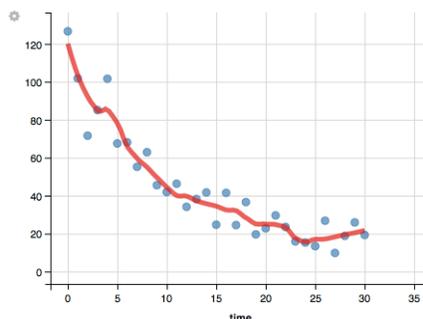


- Even though the correlation is strong, the data clearly indicate a nonlinear relationship between counts and time. To get a sense of the shape of our scatterplot, we can use *locally weighted scatterplot smoothing* (LOWESS). LOWESS connects a series of curves that are fit to small (local) subsets of the data (defined by the bandwidth/span).

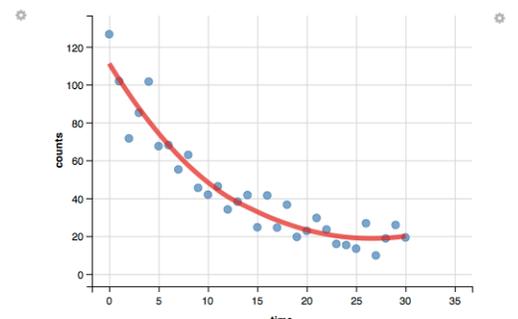
To see an animation of LOWESS in action, go to: <http://bradthiessen.com/html5/stats/m301/lowess.gif>



Bandwidth = 0.1



Bandwidth = 0.3



Bandwidth = 1.0

3. That LOWESS curve reinforces the idea that our data do not have a linear relationship.

What can we do when our data appear to have a “curved” relationship? Believe it or not, we can still use linear regression. Linear regression can include “lines” that have curved shapes.

One way to do this is to include polynomial terms in our regression model. In this Geiger counter example, we could try to fit the following models:

Linear model:  $\hat{y} = b_0 + b_1(\text{time})$

Model with quadratic term:  $\hat{y} = b_0 + b_1(\text{time}) + b_2(\text{time})^2$

Model with cubic term:  $\hat{y} = b_0 + b_1(\text{time}) + b_2(\text{time})^2 + b_3(\text{time})^3$

Each of those are considered to be linear models? Why? If you take the partial derivative of your model and the result no longer includes the unknown coefficients, then the model is considered to be linear. If, on the other hand, the partial derivative results in a function that still includes the unknown coefficients, then the model is considered to be nonlinear. Let’s take a look at the partial derivative of the model with the cubic term:

$$\frac{dy}{db_0} = 1 \quad \frac{dy}{db_1} = x \quad \frac{dy}{db_2} = x^2 \quad \frac{dy}{db_3} = x^3$$

These partial derivatives are no longer functions of the coefficients (b values), so this is a linear model (a linear combination of predictor variables).

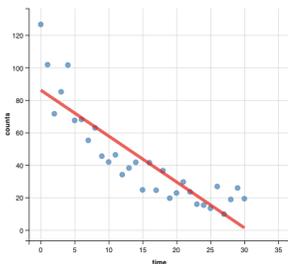
We can fit the models with the quadratic and cubic terms and compare them to the null model with no predictors:

```
lin.mod <- lm(counts ~ time, data=geiger) # Fit the linear model with one predictor
quad.mod <- lm(counts ~ time + I(time^2), data=geiger) # Include quadratic term
cub.mod <- lm(counts ~ time + I(time^2) + I(time^3), data=geiger) # Include cubic term
```

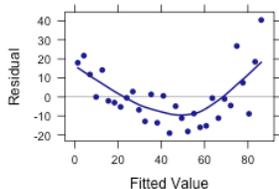
**Model: count = b<sub>0</sub> + b<sub>1</sub>(time)**

Formula:  $y = 86.1 - 2.83x$   
 $R^2 = 0.7687$   
 AIC = 256.99  
 RMSE = 14.34

Compared to null model:  
 $F = 96.397$  ( $p = 9.991e-11$ )



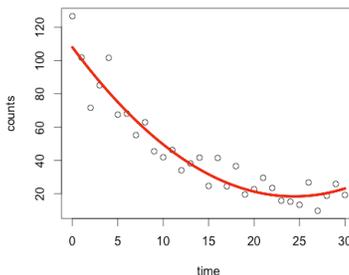
Residuals vs Fitted



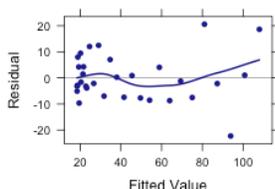
**Model: y = b<sub>0</sub> + b<sub>1</sub>(time) + b<sub>2</sub>(time)<sup>2</sup>**

Formula:  $y = 108 - 7.34x + 0.15x^2$   
 $R^2 = 0.9079$   
 AIC = 230.44  
 RMSE = 9.205

Compared to null model:  
 $F = 138.1$  ( $p = 3.143e-15$ )



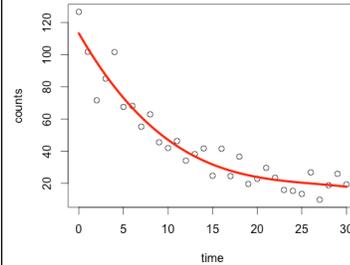
Residuals vs Fitted



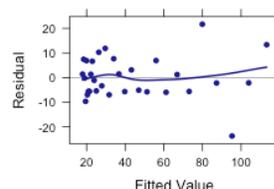
**Model: y = b<sub>0</sub> + b<sub>1</sub>(time) + b<sub>2</sub>(time)<sup>2</sup> + b<sub>3</sub>(time)<sup>3</sup>**

Formula:  $y = 113.3 - 9.65x + 0.35x^2 - 0.004x^3$   
 $R^2 = 0.915$   
 AIC = 229.97  
 RMSE = 9.007

Compared to null model:  
 $F = 96.88$  ( $p = 1.442e-14$ )



Residuals vs Fitted



4. We can compare these three models by examining the AIC values or with the omnibus F-test. Verify the calculations and interpret. From this, which model would you conclude fits the data the best?

Analysis of Variance Table

Model 1: counts ~ 1

Model 2: counts ~ time

Model 3: counts ~ time + I(time^2)

Model 4: counts ~ time + I(time^2) + I(time^3)

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	30	25769.0				
2	29	5959.5	1	19809.5	244.176	4.763e-15
3	28	2372.4	1	3587.1	44.215	3.897e-07
4	27	2190.5	1	182.0	2.243	0.1458

5. The R-squared values increased as we added higher-powered terms to our model. Does adding higher-powered terms always increase the fit of a model to a dataset? Explain.

6. Let's fit a model that includes all terms up to the 7th power:

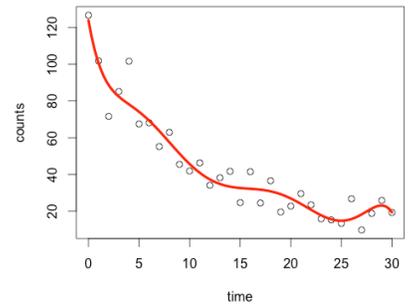
Formula:  $y = 124 - 31.6x + 9.9x^2 - 1.7x^3 + 0.15x^4 - 0.007x^5 + 0.00017x^6 - 0.0000016x^7$

$R^2 = 0.9314$

RMSE = 9.007

AIC = 231.3124

If we compare it to the model with the quadratic term, we find:



Analysis of Variance Table

Model 1: counts ~ time + I(time^2)

Model 2: counts ~ time + I(time^2) + I(time^3) + ... + I(time^6) + I(time^7)

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	28	2372.4				
2	23	1767.2	5	605.22	1.5754	0.2066

From this, what can we conclude?

7. Just like in the last activity, we can use cross-validation to help choose the best model:

<u>Average cross-validated mean square error:</u>	<u>Model</u>
888	null model
219	count = f(time)
103	count = f(time + time <sup>2</sup> )
105	count = f(time + time <sup>2</sup> + time <sup>3</sup> )
110	count = f(time + time <sup>2</sup> + time <sup>3</sup> + time <sup>4</sup> )

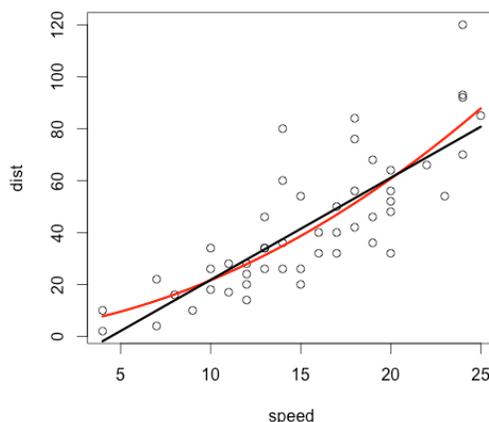
From this, what can we conclude?

8. As another quick example, we can investigate the speed and stopping distance of 50 cars. I fit models including linear, quadratic, and cubic terms and then tested each model in order:

**Analysis of Variance Table**

Model 1: dist ~ 1  
 Model 2: dist ~ speed  
 Model 3: dist ~ speed + I(speed<sup>2</sup>)  
 Model 4: dist ~ speed + I(speed<sup>2</sup>) + I(speed<sup>3</sup>)

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	49	32539				
2	48	11354	1	21185.5	91.6398	1.601e-12
3	47	10825	1	528.8	2.2874	0.1373
4	46	10634	1	190.4	0.8234	0.3689

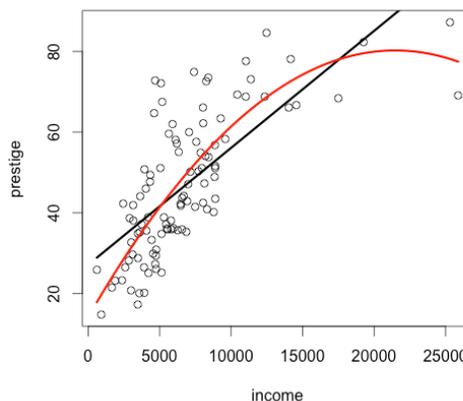


Which model would you choose to describe this data?

9. Finally, remember we predicted the prestige of occupations based on their income levels. Based on the AIC values cross-validation output, which model would you choose?

Model 1: prestige ~ 1  
 Model 2: prestige ~ income  
 Model 3: prestige ~ income + I(income<sup>2</sup>)  
 Model 4: prestige ~ income + I(income<sup>2</sup>) + I(income<sup>3</sup>)

Model 1: AIC = 873  
 Model 2: AIC = 802  
 Model 3: AIC = 784  
 Model 4: AIC = 786



<u>Average cross-validated mean square error:</u>	<u>Model</u>
154	prestige = f(income)
130	prestige = f(income + income <sup>2</sup> )
131	prestige = f(income + income <sup>2</sup> + income <sup>3</sup> )
134	prestige = f(income + income <sup>2</sup> + income <sup>3</sup> + income <sup>4</sup> )

10. So far, we've evaluated the conditions (assumptions) necessary to fit linear models, but we haven't really investigated what we can do if those conditions are not met.

If our residuals do not approximate a normal distribution, we might choose to transform our variables. If our linearity assumption is violated, we might turn to a polynomial (or nonlinear) regression model.

What do we do if we have concerns about the homogeneity of variances assumption or if our data have a few influential outliers?

We might choose to conduct a *robust* regression, using one of two methods:

- Regression with robust standard errors (when we're concerned about homoscedasticity or normal residuals)
- Robust estimation of coefficients and standard errors (when we have influential outliers)

Let's investigate the use of bootstrap methods for robust regression. With a bootstrap residuals approach, we:

- Estimate regression coefficients from the data:  $\hat{y} = b_0 + b_1x_1 + \dots$
- Calculate predicted values ( $\hat{y}$ ) and residuals for each observation ( $e = \hat{y} - y$ )
- Take all  $n$  residuals and select a sample of  $n$  of them with replacement (the bootstrap sample).
- Using those sampled residuals, calculate new Y values ( $y^* = \hat{y} + e$ )
- Now run a regression using your original x variable and the new  $y^*$  variable values
- Repeat steps c-e many times (say, 10,000 times)

Now that we have 10,000 estimates of our regression coefficients, we can estimate their standard errors by simply calculating the standard deviation of all our coefficient estimates. Likewise, we can find the lowest and highest 2.5% of the coefficient estimates to estimate a 95% confidence interval for each.

To read about this technique, check out either of the following:

<http://socserv.mcmaster.ca/jfox/Books/Companion/appendix/Appendix-Bootstrapping.pdf>

[http://www.sagepub.com/upm-data/21122\\_Chapter\\_21.pdf](http://www.sagepub.com/upm-data/21122_Chapter_21.pdf)

Let's try this out on our prestige data. We'll model prestige as a function of income, education, and %women:

	<b>Linear Model</b>		<b>Bootstrap Method</b>	
	<u>Coefficient</u>	<u>Standard Error</u>	<u>Coefficient</u>	<u>Standard Error</u>
(intercept)	-6.794334	3.239089	-6.804227	3.146723
Income	0.001314	0.000278	0.001317	0.000274
Education	4.186637	0.388701	4.188170	0.379537
%women	-0.008905	0.030407	-0.009071	0.029862

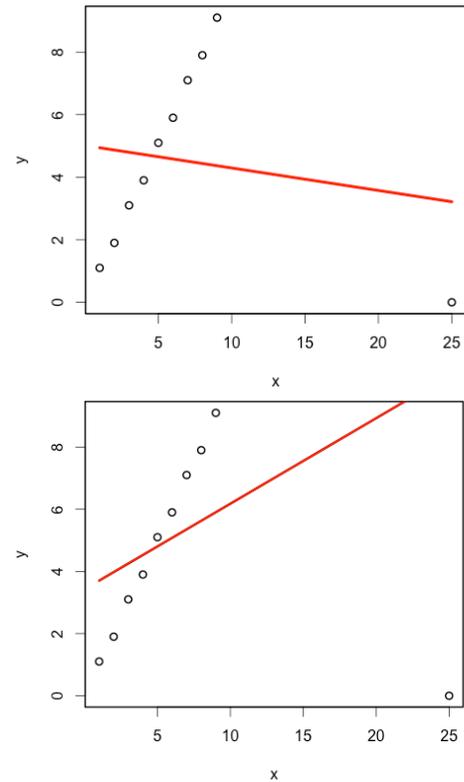
Notice the bootstrap coefficients are slightly biased (compared to our original model) and the standard errors differ. What's the consequence of having different values for these standard errors?

11. Let's take a different approach to bootstrapping a regression. We'll start with a fictitious dataset that has a clear outlier. When we fit a linear model to the data, we get what's pictured to the right.

That outlier on the bottom-right obviously had a significant impact on our estimates of the regression coefficients. To mitigate the effect of that outlier, we could choose to:

- Take a random sample of  $n$  observations with replacement from our data.
- Estimate the regression coefficients for this bootstrap sample.
- Repeat this process many times to end up with lots of estimated coefficients
- Use the mean (or median) of those bootstrap coefficients

The bootstrap regression line is pictured to the right. While it's still not a great fit, it's markedly better than the original.



Let's see how this bootstrap cases approach works on our prestige dataset. Below, I've pasted the coefficients using ordinary least squares and using the bootstrap method. Once again, notice that the coefficients and standard errors differ slightly.

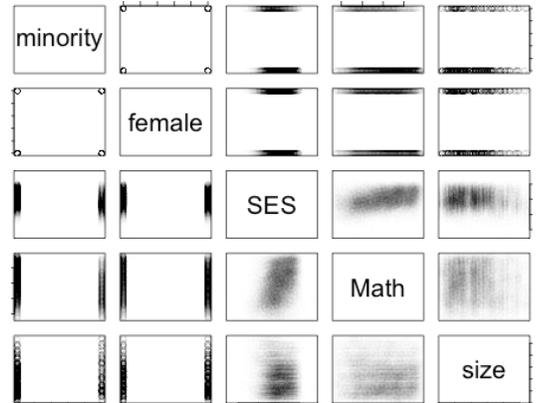
	<b>Linear Model</b>		<b>Bootstrap Method</b>	
	<u>Coefficient</u>	<u>Standard Error</u>	<u>Coefficient</u>	<u>Standard Error</u>
(intercept)	-6.794334	3.239089	-6.715968	3.227395
Income	0.001314	0.000278	0.001423	0.000445
Education	4.186637	0.388701	4.100725	0.472782
%women	-0.008905	0.030407	-0.003743	0.037316

What assumptions did we make with the ordinary least squares regression? What assumptions did we make using the bootstrap method?

Scenario: The National Center for Education Statistics (NCES) is mandated to "collect and disseminate statistics and other data related to education in the United States." To this end, it has initiated several large scale studies in which a cohort is studied at regular intervals over several years. The High School and Beyond (HSB) study tracked achievement and social aspects of the 1980 sophomore & senior classes.

Our dataset contains the following variables for 7,185 students from 160 different high schools:

- schid: school ID number
- minority: 0 = no; 1 = yes
- female: 0 = no; 1 = yes
- ses: socioeconomic status of the student (z-score)
- **mathach: math achievement score (z-score)**
- size: number of students in school
- schtype: school type (0 = public; 1 = private)
- meanses: socioeconomic status of the school



We'll focus on **mathach** as our outcome variable.

Data: <http://www.bradthiessen.com/html5/data/hsb.csv>

12. The scatterplot shows math achievement is associated with socioeconomic status. We can fit a linear model:

**Model:**  $\text{mathach} = b_0 + b_1(\text{ses})$

Formula:  $y = 0 + 0.361x$

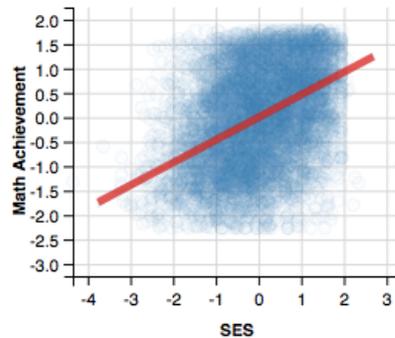
$R^2 = 0.13$

RMSE = 0.933

AIC = 19393.35

Comparison to null model:

$F = 1075$  ( $p < 2e-16$ )



From this, what can we say about the relationship between SES and math achievement?

Keep in mind our variables are standardized (z-scores).

13. In fitting that line through the scatterplot, we assume the relationship between X and Y is the same across all values of Y. In other words, we assume a 1 standard deviation increase in SES is associated with a 0.36 standard deviation increase in math achievement for all students (regardless of how high or low the students math achievement is).

Might we expect SES to have more or less of an impact on extremely low- or high-achieving students? Maybe. To investigate this, we can use **quantile regression**.

Recall the median is the 2-quantile (50th percentile). We could run a quantile regression for the 50th percentile.

**Linear Regression**

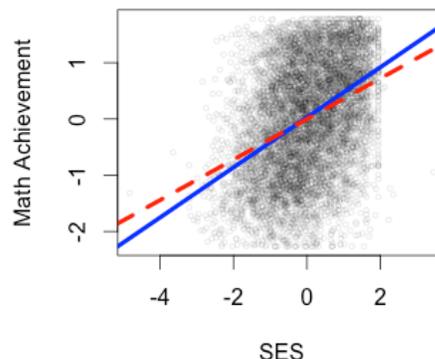
**Model:**  $\text{mathach} = b_0 + b_1(\text{ses})$

Formula:  $y = 0 + 0.361x$

**Quantile Regression for median**

**Model:**  $\text{median}(\text{mathach}) = b_0 + b_1(\text{ses})$

Formula:  $y = 0.0295 + 0.4454x$

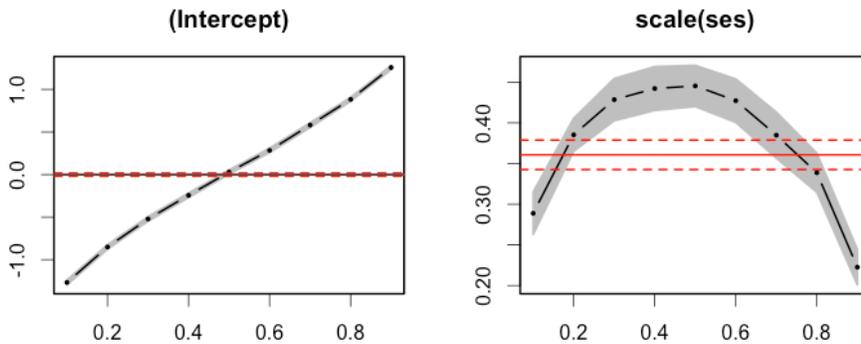


Interpret the coefficients of this quantile regression line.

14. Median regression can be useful (especially when dealing with outliers), but we're more interested in determining if the relationship between SES and math achievement differ across levels of math achievement.

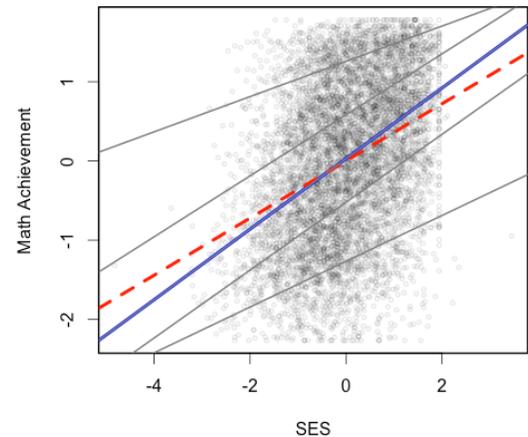
To investigate this, we can run a quantile regression for as many quantiles as we want (e.g., the 10th, 20th, 30th, ..., 80th, and 90th percentiles).

Rather than listing out the coefficients for all 9 regression model, we can display the magnitude of the coefficients across each of the 10 deciles.



The red line shows the coefficients for our simple linear regression model (along with confidence bands). The black lines show the coefficient estimate across different percentiles of math achievement (along with grey confidence bands). From this, what can we conclude about the relationship between SES and math achievement?

15. We can also display these quantile regression lines on the scatterplot. To the right, I've plotted the regression lines for the 10th, 30th, 50th, 70th, and 90th percentiles of math achievement. Do these results match the graphs displayed above?



16. It appears as though the relationship between math achievement and SES is strongest at the median math score (where it has the largest slope of 0.4454). At the 25th percentile, the slope is only 0.4058.

Is there a statistically significant difference between those two slopes? Let's compare regression models:

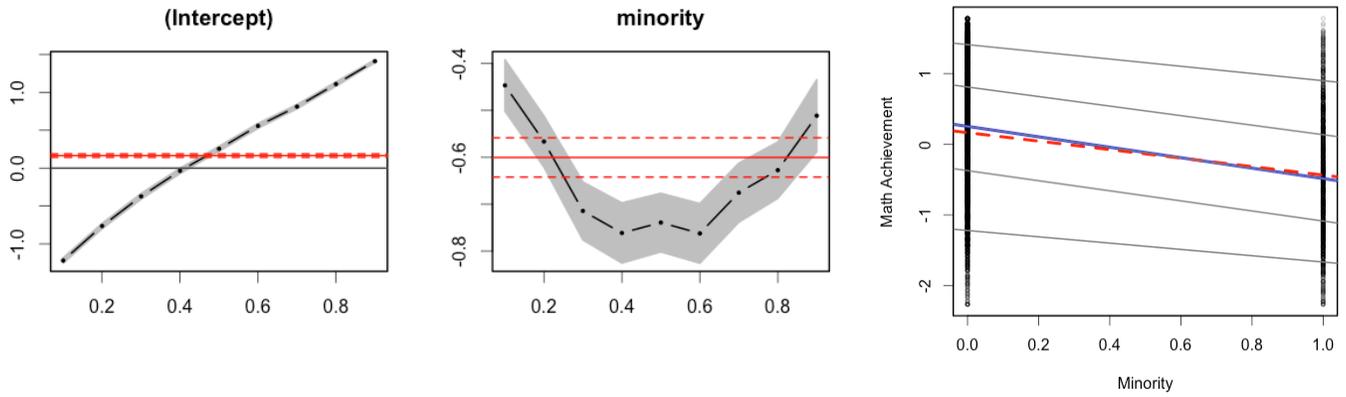
**Quantile Regression Analysis of Deviance Table**

```
Model: scale(mathach) ~ scale(ses)
Joint Test of Equality of Slopes: tau in { 0.25 0.5 }
```

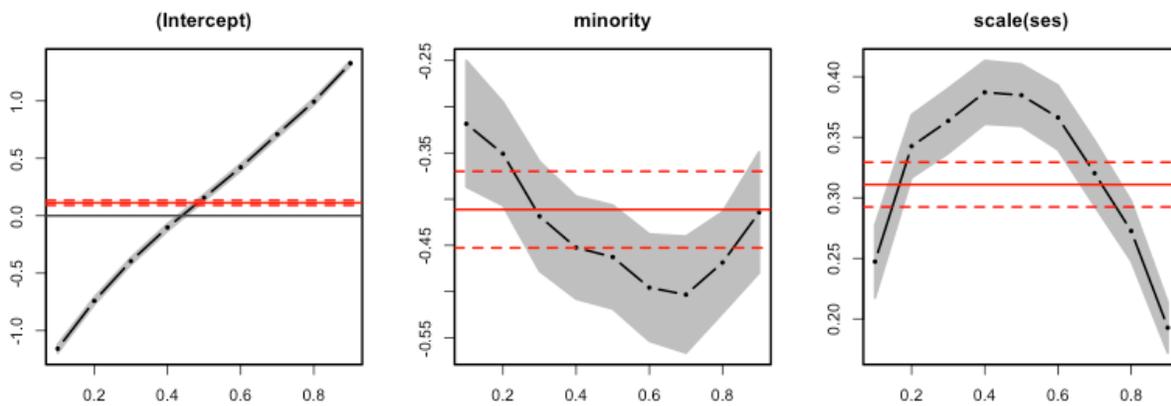
```
  Df Resid Df F value Pr(>F)
1 1 14369 7.45 0.0064 **
```

What can we conclude from this?

17. We've investigated the math achievement gap associated with differences in socioeconomic status. Does the achievement gap for minority students also differ across levels of math achievement? Interpret the output.



18. We can include both predictors (SES and minority) and run a multiple quantile regression analysis. Interpret.





Interpret the slope coefficient. Then, explain why this coding scheme is a bad idea.

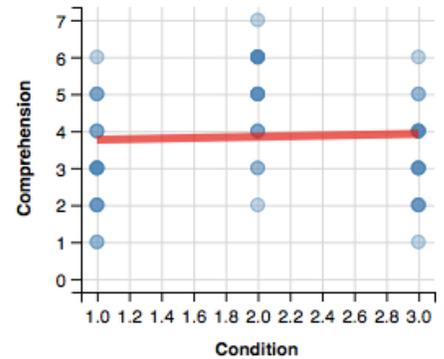
**Model: comprehension =  $b_0 + b_1(\text{condition code})$**

Formula:  $y = 3.68421 + 0.07895x$

$R^2 = 0.001828$

RMSE = 1.534

F = 0.1007 (p = 0.7522)



20. If we want to include a categorical predictor in our regression model, we'll need to convert that categorical predictor to a factor variable (or series of dummy variables).

Dummy variables take values of 0 or 1 to indicate the absence or presence of a categorical effect. In this example, we could convert the 3 condition groups into 3 dummy variables:

- Dummy variable #1 = 1 if the condition is **after** (and equals zero for the before and none categories)
- Dummy variable #2 = 1 if the condition is **before** (and equals zero for the after and none categories)
- Dummy variable #3 = 1 if the condition is **none** (and equals zero for the before and after categories)

These dummy variables are displayed in the table on the previous page.

If we enter these dummy variables and fit our regression model ( $\hat{y} = b_0 + b_1x_1 + b_2x_2 + b_3x_3$ ), we get:

**Coefficients: (1 not defined because of singularities)**

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	3.3684	0.3035	11.097	1.51e-15
x1	-0.1579	0.4293	-0.368	0.714436
x2	1.5789	0.4293	3.678	0.000542
x3	NA	NA	NA	NA

Why did we get an error message?

21. Including all 3 dummy variables gives us a perfect collinearity problem. All the information we need about the condition groups is contained within the first 2 dummy variables:

- $x_1 = 1$  if the condition is **after** (and equals zero for the before and none categories)
- $x_2 = 1$  if the condition is **before** (and equals zero for the after and none categories)

To demonstrate this, identify the condition (after, before, or none) for each of the following:

<u>x1</u>	<u>x2</u>	<u>Condition</u>
1	0	_____
0	1	_____
0	0	_____

22. Let's run our regression again, this time using only the first two dummy variables:  $\hat{y} = b_0 + b_1x_1 + b_2x_2$   
 Interpret this output. What do the coefficients represent?

```

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)   3.3684    0.3035  11.097 1.51e-15
x1            -0.1579    0.4293  -0.368 0.714436
x2             1.5789    0.4293   3.678 0.000542
---
Residual standard error: 1.323 on 54 degrees of freedom
Multiple R-squared:  0.2705, Adjusted R-squared:  0.2435
F-statistic: 10.01 on 2 and 54 DF,  p-value: 0.0002002
  
```

23. The ANOVA summary table for this regression model (using dummy variables) corresponds with the ANOVA summary table we calculated in way back in lesson #3.

**Original ANOVA summary table**

Source	SS	df	MS	MSR (F)
Treatment	35.053	2	17.5263	10.012
Error	94.526	54	1.7505	p = 0.0002
Total	129.579	56	MS <sub>total</sub>	η <sup>2</sup> = 0.2705

**Regression Analysis**

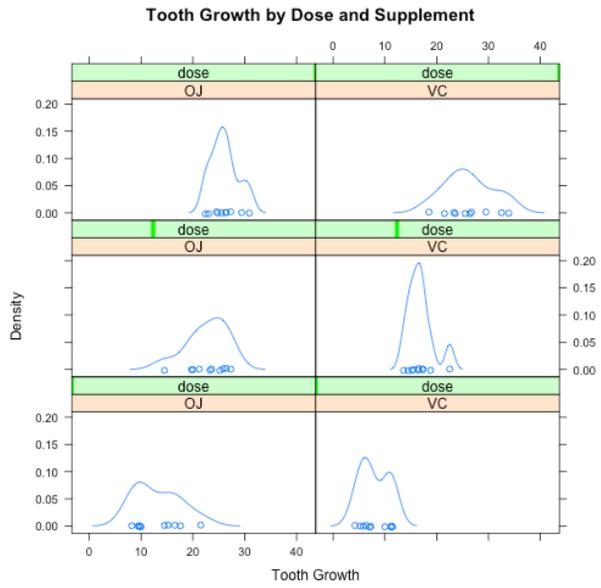
Source	SS	df	MS	MSR (F)	
model	35.053	2	17.5263	10.012	p=0.002
x1	11.369	1	11.369	6.494	p=0.014
x2	23.684	1	23.684	13.530	p=0.001
Error	94.526	54	1.7505		
Total	129.579	56	MS <sub>total</sub>		

24. We can also conduct an AxB ANOVA as a regression analysis.  
 To demonstrate, let's use the guinea pig tooth growth data we may have investigated back in the first unit.

This study investigated tooth growth in guinea pigs as a function of the type and dose of vitamin C. Guinea pigs were given a low, medium, or high dose of vitamin C either through orange juice (OJ) or a vitamin C supplement (VC).

Here's a quick summary of our data:

supp	dose	n	mean	sd	
1	OJ	0.5	10	13.23	4.459709
2	OJ	1	10	22.70	3.910953
3	OJ	2	10	26.06	2.655058
4	VC	0.5	10	7.98	2.746634
5	VC	1	10	16.77	2.515309
6	VC	2	10	26.14	4.797731



We can convert our dose and supplement variables into dummy variables:

Guinea Pig	Original data			Dummy coding		
	y = tooth growth	Supplement	Dose	Supp.Code	Dose1	Dose2
1	4.2	OJ	Low	0	1	0
2	11.5	OJ	Medium	0	0	1
3	7.3	OJ	High	0	0	0
4	5.8	VC	Low	1	1	0
5	6.4	VC	Medium	1	0	1
6	10.0	VC	High	1	0	0
...	...	...	...	...	...	...

We can then fit a linear model, including the interaction terms.

$$\hat{y} = b_0 + b_1(\text{supp.code}) + b_2(\text{dose}_{low}) + b_3(\text{dose}_{med}) + b_4(\text{supp.code})(\text{dose}_{low}) + b_5(\text{supp.code})(\text{dose}_{med})$$

Fitting the model results in the following parameter estimates:

**Coefficients:**

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	13.230	1.148	11.521	3.60e-16
suppVC	-5.250	1.624	-3.233	0.00209
dose1	9.470	1.624	5.831	3.18e-07
dose2	12.830	1.624	7.900	1.43e-10
suppVC:dose1	-0.680	2.297	-0.296	0.76831
suppVC:dose2	5.330	2.297	2.321	0.02411

Interpret this output.

25. Compare the AxB ANOVA summary table with the ANOVA summary table from this regression analysis.

AxB ANOVA					
Source	SS	df	MS	MSR (F)	
supplement	205.4	1	205.4	15.572	p=0.0002
dose	2426.4	2	1213.2	92.000	p<0.00001
interaction	108.3	2	54.2	4.107	0.02186
Error	712.1	54	13.2		
Total	3452.2	59	MS <sub>total</sub>		

Regression					
Source	SS	df	MS	MSR (F)	
supplement	205.4	1	205.4	15.572	p=0.0002
dose	2426.4	2	1213.2	92.000	p<0.00001
supp:dose	108.3	2	54.2	4.107	0.02186
Error	712.1	54	13.2		
Total	3452.2	59	MS <sub>total</sub>		